Log Concave Coupling for Sampling from Neural Net Posterior Distributions

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Outline

- Neural Net Model and Approximation
 - Target f with variation $V_L(f)$ when represented with L layers
 - Approximation f_{M,L} with L layers and M subnetworks
 - Approximation Accuracy $||f f_{M,L}||^2 \le \frac{V_L^2(f)}{M}$
- Neural Net Estimation and Risk
 - Estimate weights w, variation V, num subnets M, depth L
 - Constrained Least Squares: computational open problem
 - Bayes Predictive Mean Estimators: MCMC. Is it rapid?
 - Risk with sample size N and input dimension d

$$E||\hat{f} - f||^{2} \leq \frac{V_{L}^{2}(f)}{M} + \frac{M\log(2d) + ML}{N}$$
$$E||\hat{f} - f||^{2} \leq V_{L}(f)\sqrt{\frac{\log(2d) + L}{N}}$$

Outline: Continued

- Log Concave Coupling for Bayesian Computation
 - Focus attention on single hidden-layer network models
 - Prior density $p_0(w)$: Uniform on ℓ_1 constrained set
 - Posterior p(w): Multimodal. No known direct rapid sampler
 - Coupling $p(\xi|w)$: cond indep Gaussian auxiliary variables $\xi_{i,m}$ with mean $x_i \cdot w_m$ for each observation *i* and neuron *m*
 - Conditional $p(w|\xi)$ always log-concave
 - Marginal $p(\xi)$ and its score $\nabla \log p(\xi)$ rapidly computable
 - *p*(ξ) is log concave when the number of parameters *Md* is large compared to the sample size *N*
 - Langevin diffusion and other samplers are rapidly mixing
 - With a draw from p(ξ) followed by a draw from p(w|ξ) we obtain a draw from the desired posterior p(w)

Variation and Approximation with a Dictionary G

- Variation with respect to a dictionary
 - Dictionary G of functions g(x, w), each bounded by 1
 - Consider linear combinations $\sum_{j} c_{j} g(x, w_{j})$
 - Control the sum of abs values of the weights $\sum_{i} |c_{i}| \leq V$
 - \mathcal{F}_V = closure of signed convex hull of functions V g(x, w)
 - Variation $V_G(f)$ = the infimum of V such that $f \in \mathcal{F}_V$.
- Approximation accuracy
 - Function norm square $||f g||^2$ in $L_2(P_X)$
 - *M* term approximation: $f_M(x) = \sum_{m=1}^{M} c_m g(x, w_m)$
 - Approximation error: $||f f_M||^2 \le \frac{V(f)^2}{M}$
 - Trivial existence proof: Bernoulli, Hilbert, Maurey, Pisier, Barron 93
 - Greedy approximation proof: Jones, Barron 93
 - Outer weights c_m may equal $\pm \frac{V}{M}$
 - Approximation error better than $\frac{V^2}{M}$ is *NP*-hard (Vu 97)
 - Rate $\frac{1}{M}$ is dimension independent

Models

- Approximation error for $f_M(x) = \sum_{m=1}^M c_m g(x, w_m)$ $||f - f_M||^2 \le \frac{V_G^2(f)}{M}$
- Algorithmic Terminology

Sparse Term Selection, Variable Selection, Basis Selection, Forward Stepwise Regression, Relaxed Greedy Algorithm, Orthogonal Matching Pursuit, Frank Wolf Alg, Greedy Bayes

Models

Projection Pursuit (ridge functions), MARS (splines), MAPS (polynomials), Prony (sinusoids), Wavelets, Ridgelets, Random Forests (regression trees)

Network Models

Single Hidden-Layer Nets, Multi-Layer Networks, Deep Nets, Adaptive Learning Networks, Residual Networks

 Network Units (neurons) Sigmoids, Rectified Linear Units (ReLU), Polynomials, compositions thereof

Multi-Layer Neural Network Model

- Multi-Layer Net: Layers L, input x in $[-1, 1]^d$, weights w
- Activation function: $\psi(z)$.
 - Rectified linear unit (ReLU): $\psi(z) = (z)_+$
 - Twice differentiable unit: sigmoid, smoothed ReLU, squared ReLU
- Paths of linked nodes: $\underline{j} = j_1, j_2, ..., j_L$.
- Path weight: $W_{\underline{j}} = w_{j_1,j_2}w_{j_2,j_3}\cdots w_{j_{L-1},j_L}$.
- Function representation:

 $f(x, c, w) = \sum_{j_L} c_{j_L} \psi(\sum_{j_{L-1}} w_{j_{L-1}, j_L} \psi(\dots \psi(\sum_{j_1} w_{j_1, j_2} x_{j_1}) \dots))$

- Network Variation:
 - Internal: Sum abs. values of path weights set to 1.
 - External: $\sum_{j} |c_{j}| \leq V$
 - Variation: V_L(f) = infimum of such V to represent f
 - Single Hidden-Layer Case: $V_1(f) \leq \int |\omega|_1^2 |\tilde{f}(\omega)| d\omega$ spectral norm
 - Class $\mathcal{F}_{L,V}$ of functions f with $V_L(f) \leq V$
- Interests: Approx, Metric Entropy, Stat. Risk, Computation

Complexity, Metric Entropy, Statistical Risk

Gaussian complexity approach to bounding risk

• Function class restricted to data:

 $\mathcal{F}^n = \{f(x_1), f(x_2), \ldots, f(x_n) : f \in \mathcal{F}\}$

Gaussian Complexity:

 $C(A) = (1/\sqrt{n})E_Z[\sup_{a \in A} a \cdot Z]$ for $Z \sim N(0, I) \ A \subset R^n$

Complexity of Neural Nets:

 $C(\mathcal{F}_{L,V}^n) \leq V\sqrt{2\log 2d + 2L\log 2}$

for ψ Lipshitz 1 via Fernique Gaussian comparison ineq, Klusowski, B. 2020 (cf Neshabur et al 15, Golowich et al 18)

- Gaussian complexity provides control of
 - Metric Entropy:

$$\log |Cover(\mathcal{F}_{L,V}, \delta)| \leq \frac{16C^2(\mathcal{F}_{L,V})}{\delta^2}$$

• Stat Risk of Constrained Least Squares:

$$E||\hat{f}-f||^2 \leq \frac{8C(\mathcal{F}_{L,V})}{\sqrt{n}}$$

Minimum Description Length and Bayes predictive risk

- Minimum Description Length; optimize penalized likelihood
 - Least squares with suitable penalization for choice of *M*, *V*
 - $||\hat{f} f||^2$ risk via Renyi-Battacharya risk inequality: B, Luo 08
 - Index of Resolvability: ApproxError + Complexity/N
- Predictive Bayes and its cumulative risk control
 - Predictive density $\hat{p}_n(y|x) = \int p(y|x, w) p(w|x^n, y^n) dw$
 - Predictive mean $\hat{f}_n(x) = \int f(x, w) p(w|x^n, y^n) dw$
 - Predictive evaluations for $Y_{n+1} = y$ when $X_{n+1} = x$
 - Inf Thy chain rule for cumulative Kullback risk: B. 86,98

$$\frac{1}{N}\sum_{n=0}^{N-1} ED(P_{Y|X}^*||\hat{P}_{Y|X}^n) = \frac{1}{N}D(P_{Y^N,X^N}^*||P_{Y^N,X^N})$$

- Controls data compression redundancy as well as the risk
- Index of Resolvability:

ApproxError + $\frac{1}{N} \log[1 / PriorProb(ApproxSet)]$

• Used in Yang, B (98) minimax risk characterization

$$E||f - \hat{f}_{N}||^{2} \leq \min_{\delta} \left\{ \delta^{2} + \frac{1}{N} \mathsf{log}|\mathsf{Cover}(\mathcal{F}_{L,V}, \delta)| \right\} \leq \frac{\mathsf{BC}(\mathcal{F}_{L,V})}{\sqrt{N}}$$

Arbitrary Sequence Predictive Bayes Regret

- On-line learning
- Arbitrary-sequence regret for predictive Bayes

$$\frac{1}{N}\sum_{n=1}^{N}(Y_n - \hat{f}_{n-1}(X_n))^2 - \frac{1}{N}\sum_{n=1}^{N}(Y_n - f(X_n))^2$$

• Bound hold of the same form, uniformly over X^N , Y^N ,

 $Regret_N \leq Approx Error + \frac{1}{N} \log \frac{1}{PriorProb(Approx Set)}$

• Specialization of bound to the case of functions f in F_{1,V}

$$\textit{Regret}_{N} \leq V rac{\sqrt{\textit{logd}}}{\sqrt{N}}$$

Taking expectation controls

$$\frac{1}{N}\sum_{n=1}^{N} E||f - \hat{f}_{n-1}||^2$$

• Estimator $\hat{f}_N(x) = \frac{1}{N} \sum_{n=1}^N \hat{f}_{n-1}$ also has this bound

$$E[||\hat{\hat{f}}_N - f||^2] \leq V rac{\sqrt{\log d}}{\sqrt{N}}$$

Bayesian Computation for Neural Net

- Sample sizes: $n \le N$
- Data^{*n*} = ((X_i, Y_i) for i = 1, 2, ..., n), with X_i in $[-1, 1]^d$
- Natural yet optional statistical assumption:
 (X_i, Y_i) independent P_{X,Y}, with target f(x) = E[Y | X = x]
 - Not needed for Bayesian computation statements
 - Not needed for online learning bounds
- Single hidden-layer network model: f(x, w)

 $f_M(x,\underline{w}_1,\ldots\underline{w}_M) = \frac{V}{M}\sum_{m=1}^M \psi(\underline{w}_m\cdot x_i)$

- each \underline{w}_m in symmetric simplex $S_1^d = \{w : \sum_{j=1}^d |w_j| \le 1\}$
- Prior: $p_0(\underline{w})$ makes \underline{w}_m independent uniform on S_1^d
- Likelihood: exp $\{-\beta g(w)\}$ where $g(w) = \frac{1}{2} \sum_{i=1}^{n} (Y_i - \frac{V}{M} \sum_{m=1}^{M} \psi(x_i \cdot w_m))^2$
- Posterior: $p(w) = p_0(w) \exp\{-\beta g(w) \Gamma(\beta)\}$
- Bayesian Computation: Estimate $\hat{f}(x) = \int f(x, w)p(w)dw$ by drawing independent samples from p(w) and averaging f(x, w)

Hessian of the Minus Log Likelihood

• Log 1/Likelihood = $\beta q(w)$ • Gradient score(w) = $\beta \nabla g(w)$ • Hessian = $\beta H(w) = \beta \nabla \nabla' g(w)$ • Squared error loss: g(w) $\frac{1}{2}\sum_{i=1}^{n}(res_i(w))^2$ where $res_i(w) = Y_i - \frac{V}{M}\sum_{m=1}^{M}\psi(x_i \cdot w_m)$ • Gradient: $\nabla_{w_m} g(w)$ for block m $-\frac{V}{M}\sum_{i=1}^{n} res_i(w)\psi'(x_i \cdot w_m)x_i$ • Hessian: $H_{w_k,w_m}(w) = \nabla_{w_k} \nabla'_{w_m} g(w)$ for block k, m $\frac{V^2}{M^2} \sum_{i=1}^{n} \psi'(\mathbf{X}_i \cdot \mathbf{W}_k) \psi'(\mathbf{X}_i \cdot \mathbf{W}_m) \mathbf{X}_i \mathbf{X}_i'$ $-\frac{V}{M}\sum_{i=1}^{n} res_i(w)\psi''(x_i \cdot w_m)x_ix_i'\mathbf{1}_{k=m}$ • Quadratic form: a'H(w)a, where a has blocks $a_m 1 \le m \le M$ $\frac{V^2}{M^2}\sum_{i=1}^{n}\left(\sum_{m=1}^{M}\psi'(x_i\cdot w_m)a_m\cdot x_i\right)^2$ $-\frac{V}{M}\sum_{i=1}^{n} res_i(w) \sum_{m=1}^{M} \psi''(x_i \cdot w_m)(a_m \cdot x_i)^2$

- p(w) is not log-concave; that is, g(w) is not convex
 The first term is positive definite, the second term is not
- No clear reason for gradient methods to be effective

Log Concave Coupling

- Auxiliary Random Variables $\xi_{i,m}$ chosen conditionally indep
- Normal with mean $x_i \cdot w_m$, variance $1/\rho$, with $\rho = \beta c V/M$
- Conditional density:

 $p(\xi|w) = (\rho/2\pi)^{Mn/2} exp\{-\frac{\rho}{2} \sum_{i=1}^{n} \sum_{m=1}^{M} (\xi_{i,m} - x_i \cdot w_m)^2\}$

- Multiplier $c = c_{Y,V} = \max_i |Y_i| + V$ exceeds $|res_i(w)|$ for all w
- Activation second derivative: $|\psi''(z)| \le 1$ for $|z| \le 1$
- Joint density: $p(w, \xi) = p(w)p(\xi|w)$
- Reverse conditional density:

 $\rho(w|\xi) = \rho_0(w) \exp\{-\beta g_{\xi}(w) - \Gamma_{\xi}(\beta)\}$

• Conditional log 1/Likelihood = $\beta g_{\xi}(w)$ with

$$g_{\xi}(w) = g(w) + \frac{1}{2} \frac{V}{M} c \sum_{i=1}^{n} \sum_{m=1}^{M} \left(x_i \cdot w_m - \xi_{i,m} \right)^2$$

- Modifies Hessian $a'H_{\xi}(w)a$ with new positive def second term $\frac{V}{M}\sum_{i}\sum_{m} [c + res_{i}(w)\psi''(x_{i} \cdot w_{m})](a_{m} \cdot x_{i})^{2}$
- $p(w|\xi)$ is log concave in w for each ξ
- Efficiently sample. MCMC theory, Lovasz, Kannan, Vempala,...

Marginal Density and Score of the Auxiliary Variables

• Auxiliary variable density function:

 $p(\xi) = \int p(w,\xi) dw$

Integral of a log concave function of w

• Rule for Marginal Score:

 $\nabla \log 1/p(\xi) = E[\nabla \log 1/p(\xi|w) | \xi]$

Normal Score: linear

 $\partial_{\xi_{i,m}} \log 1/p(\xi|w) = \rho\left(\xi_{i,m} - x_i \cdot w_m\right)$

Marginal Score:

 $\partial_{\xi_{i,m}} \log 1/p(\xi) = \rho\left(\xi_{i,m} - E[x_i \cdot w_m \,|\, \xi]\right)$

- Efficiently compute ξ score by Monte Carlo sampling of w|ξ
- Permits Langevin stochastic diffusion: with gradient drift $d \xi(t) = \frac{1}{2} \nabla \log p(\xi(t)) dt + d B(t)$ converging to a draw from the invariant density $p(\xi)$
- Lyapunov function identification $e^{\alpha ||\xi||^2}$ as in Hairer (21) reveals exponential convergence $||p_t p||_1 \le e^{-t/\tau}$
- What is the size of \(\tau > 0\)?

Hessian of log $1/p(\xi)$. Is $p(\xi)$ log concave?

• Hessian of $\log 1/p(\xi)$, an *nM* by *nM* matrix

$$\tilde{H}(\xi) = \nabla \nabla' \log 1/\rho(\xi) = \rho \left\{ I - \rho \operatorname{Cov} \begin{bmatrix} X_{W_1} \\ \cdots \\ X_{W_M} \end{bmatrix} \right\}$$

- Hessian quadratic form for unit vectors a in \mathbb{R}^{nM} with blocks a_m $a'\tilde{H}(\xi)a = \rho \{1 - \rho \ Var[\tilde{a} \cdot w|\xi]\}$ where $\tilde{a} = \begin{bmatrix} \chi' a_1 \\ \chi' a_2 \end{bmatrix}$ has $||\tilde{a}||^2 \le n d$
- Requires variance of $\tilde{a} \cdot w$ using the log-concave $p_{\beta}(w|\xi)$
- More concentrated, smaller variance, than with the prior?
- Counterpart using the prior

 $\rho \left\{ 1 - \rho \, Var_0 [\tilde{a} \cdot w] \right\}$

- Use $Cov_0(w_m) = \frac{2}{(d+2)(d+1)}I$ and $\rho = \beta cV/M$ to see its at least $\rho \left\{ 1 \frac{2\beta cVn}{M(d+2)} \right\}$
- Constant β chosen such that $\beta cV \leq 1/4$
- Strictly positive when number param Md exceeds sample size n
- Hessian $\geq (\rho/2)I$. Strictly log concave

Rapid Convergence of Stochastic Diffusion

• Recall the Langevin diffusion

 $d\xi(t) = \frac{1}{2}\nabla \log p(\xi(t)dt + dB(t))$

- There are time-discretizations (e.g. Metropolis adjusted)
- Natural initialization choice $\xi(0)$ distributed $N(0, (1/\rho)I)$
- Bakry-Emery theory (initiated in 85)
- Strong log concavity yields rapid Markov proc. convergence
- In particular, in the stochastic diffusion setting

 $abla
abla' \log 1/p(\xi) \ge (
ho/2)I$

yields exponential conv. of relative entropy (Kullback distance) $D(p_t || p) \leq e^{-t\rho/2} D_0$

 In particular, the time required for small relative entropy is controlled by τ = 2/ρ, here equal to 2M/(βcV)

Is $p(\xi)$ log concave?

- Recap: quadratic form in Hessian of log 1/p(ξ)
 a' H
 [´](ξ)a = ρ {1 − ρ Var[ã ⋅ w|ξ]}
- Suppose p(w|ξ) has smaller variance than with the prior. Then, when *Md* exceeds *n*, this Hessian is strictly positive def, that is, p(ξ) is strictly log concave
- Other available controls on the variance $Var[\tilde{a} \cdot w|\xi] \leq \int (\tilde{a} \cdot w)^2 \exp\{-\beta g_{\xi}(w) - \Gamma_{\xi}(\beta)\} p_0(w) dw$
- Hölder's inequality

 $< [E_0[(\tilde{a} \cdot w)^{2k}]]^{1/k} \exp\{\frac{k-1}{k} \Gamma_{\xi}(\frac{k}{k-1}\beta) - \Gamma_{\xi}(\beta)\}$

- Deduce a choice of k such that ρVar[ã · w|ξ] is less than 1, for all Md at least a suitable power of n
- Carried out this agenda in a related greedy Bayes model (next)

Greedy Bayes

- Initialize $\hat{f}_{n,0}(x) = 0$
- Given previous neuron fits, iterate k, for each n $f_{n\,k}(x, w) = (1 - \alpha)f_{n\,k-1}(x) + \lambda \psi(w \cdot x)$
- $\alpha = 1/\sqrt{N}$ and $\lambda = V\alpha$ are suitable.
- Form the iterative squared error g(w) $g_{n,k}(w) = \frac{1}{2} \sum_{i=1}^{n-1} (y_i - f_{i,k}(x_i, w))^2$ Again Hessian has a not necessarily positive definite part $-\lambda \sum_{i=1}^{n-1} r_{i,k-1} \psi''(w \cdot x_i) x_i x'_i$
- Associated greedy posterior p_{n,k}(w) proportional to p₀(w) exp{-βg_{n,k}(w)}
- Update $f_{n,k}$ replacing $\psi(w \cdot x)$ with its posterior mean
- Estimate by sampling from the greedy posterior

Log Concave Coupling for Greedy Bayes

- For the moment, fix *n*, *k*
- Again $p(w) = p_0(w) \exp\{-\beta g(w)\}$
- Coupling random variables $\xi_i \sim N(x_i \cdot w, 1/\rho)$ with $\rho = c\lambda\beta$
- Joint density $p(w, \xi)$ with logarithm $-\beta g(w, \xi)$ built from $\beta g(w) + \frac{1}{2}c\lambda \sum_{i=1}^{n-1} (\xi_i - w \cdot x_i)^2$

which is convex in *w* for each ξ , so $p(w|\xi)$ is log concave

- The associated marginal is $p(\xi)$
- Hessian quadratic form $a' \nabla \nabla \log 1/p(\xi)a$

 $\rho\{\mathbf{1} - \rho Var[\tilde{\mathbf{a}} \cdot \mathbf{w}|\xi]\}$

for *a* with ||a|| = 1 and $\tilde{a} = X'a$

- Deduce $p(\xi)$ is log concave for sufficiently large d
- From which get w by a draw from $p(w|\xi)$

Variance control using Hölder's inequality

• As before $Var[\tilde{a} \cdot w|\xi]$ is not more than

 $\int (\tilde{\boldsymbol{a}} \cdot \boldsymbol{w})^2 \exp\{-\beta g_{\xi}(\boldsymbol{w}) - \Gamma_{\xi}(\beta)\} \boldsymbol{p}_0(\boldsymbol{w}) \, d\boldsymbol{w}$

where $g_{\xi}(w)$ is $g(w,\xi)$ minus its mean value at $\beta = 0$

- $\Gamma_{\xi}(w)$ is the cumulant generating function of $-g_{\xi}(w)$
- By Hölders inequality that variance is not more than
 [E₀[(ã · w)^{2k}]]^{1/k} exp{k-1/k Γ_ξ(k-1/β) − Γ_ξ(β)}
- For the first factor, for unit vectors ν $E_0[(\nu \cdot w)^{2k}] \le \frac{(2k)!}{(d+2k)\cdots(d+1)}$
- Implication

 $[E_0[(\tilde{a} \cdot w)^{2k}]]^{1/k} \le ||\tilde{a}||^2 \left(\frac{2k}{ed}\right)^2$

On the second factor from Hölders inequality

- The exponent of the second factor is $\frac{k-1}{k}\Gamma_{\varepsilon}(\frac{k}{k-1}\beta) \Gamma_{\varepsilon}(\beta)$
- It takes the form $\beta^2 Var_{\tilde{\beta}}[g_{\xi}(w)|u]/(k-1)$
- Subtracting the value at 0 we have for some \tilde{w}

 $g_{\xi}(w) - g_{\xi}(0) = w'
abla g_{\xi}(ilde w)$

- So the max square of w'∇g_ξ(w̃) bounds variance of g_ξ(w)
- Indeed a value near $(2c\lambda n)^2$ bounds that variance
- Optional page verifies this for a suitable set of *u*
- Hence the exponent of second factor not more than value near

 $4\beta^2\lambda^2c^2n^2/k$

Optional page verifying bound on $w' \nabla g_{\xi}(\tilde{w})$

• Concerning $\nabla g_{\xi}(\tilde{w})$ it is

$$-\lambda\left\{\sum_{i=1}^{n-1}\left[\operatorname{res}_{i,k-1}\psi'(\tilde{w}\cdot x_i)-\tilde{cw}\cdot x_i\right]x_i+\sum_{i=1}^{n-1}\xi_ix_i\right\}$$

- Hit with *w*, the result has magnitude not more than $2c\lambda n + \lambda \max_j |\sum_{i=1}^{n-1} \xi_i x_{i,j}|$
- With high probability, the max is not more than $\kappa \sqrt{n/\rho}$ where $\kappa = \sqrt{2 \log 2d}$
- So the max is of smaller order than the first term
- Restrict the ξ to have such bound
- Then exponent of second factor not more than value near $4\beta^2\lambda^2c^2n^2/k$

Combining the two factors

- Use $\tilde{a} = \sum_{i} a_{i} x_{i}$ with $||\tilde{a}||^{2} \leq nd$ and $\rho = c\lambda\beta$
- Combine the two factors
- Obtain ρ Var[ã · w|ξ] not more than
 cλβ nd(2k/(ed)² exp{4β²λ²c²n²/k}
- The optimal $k = 2\beta^2 \lambda^2 c^2 n^2$ yielding not more than $4(c\lambda\beta n)^5/d$
- Recall $\lambda = V\alpha = V/\sqrt{n}$
- Choose $\beta = 1/(2cV)$, choose $d \ge n^{5/2}$.
- $\rho Var[\tilde{a} \cdot w|\xi]$ is strictly less than 1 indeed (less than 1/2)
- Hence $p(\xi)$ is strictly log concave, for *d* exceeding $n^{5/2}$

Summary

- Multimodal neural net posteriors can be efficiently sampled
- Log concave coupling provides the key trick
- Requires number of parameters *Md* large compared to the sample size *N*
- Statistically accurate provided ℓ_1 controls are maintained on the parameters
- Provides the first demonstration that the class $\mathcal{F}_{1,V}$ associated with single hidden layer networks (including the class of functions with bounded L_1 spectral norm) is both computationally and statistically learnable
- A polynomial number of computations in the size of the problem is sufficient
- The approximation rate 1/M and the statistical learning rate $1/\sqrt{N}$ are independent of the dimension for this class of functions